Sc_2S_3 Structure:
A3B2_oF80_70_fh_2e-001
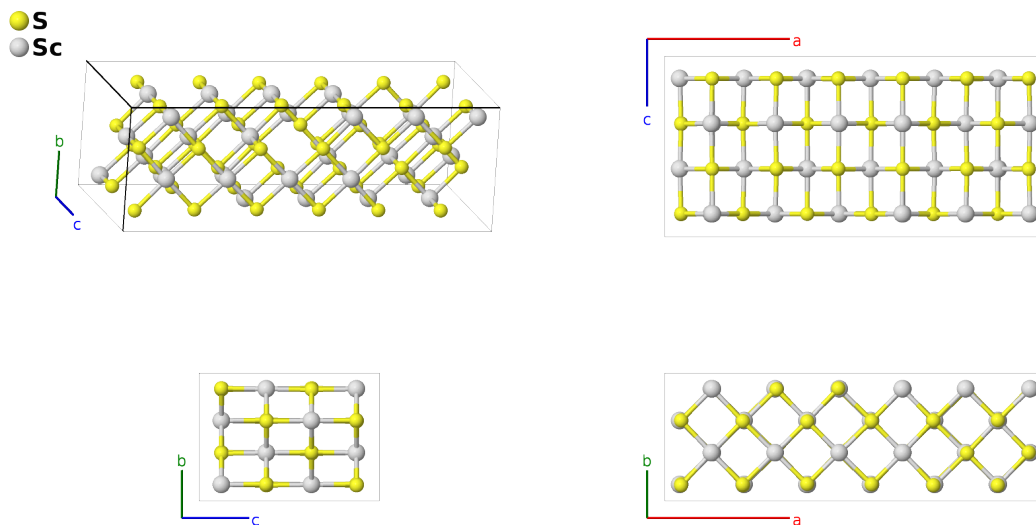
Prototype	S_3Sc_2
AFLOW prototype label	A3B2_oF80_70_fh_2e-001
ICSD	22236
Pearson symbol	oF80
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	aflow --proto=A3B2_oF80_70_fh_2e-001
	--params=$a, b/a, c/a, x_1, x_2, y_3, x_4, y_4, z_4$

Other compounds with this structure

Dy_2Se_3, Dy_2Te_3, Eu_2Se_3, Eu_2Te_3, Lu_2Se_3, Sc_2Se_3, Y_2Se_3, Y_2Te_3, Yb_2Se_3
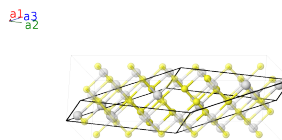
- This structure has been rotated from the orientation given by (Dismukes, 1964).

Face-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$-\left(x_1-\frac{1}{4}\right)\mathbf{a_1}+x_1\,\mathbf{a_2}+x_1\,\mathbf{a_3}$	$=$	$ax_1\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_2}$	$=$	$x_1\,\mathbf{a_1}-\left(x_1-\frac{1}{4}\right)\mathbf{a_2}-\left(x_1-\frac{1}{4}\right)\mathbf{a_3}$	$=$	$-a\left(x_1-\frac{1}{4}\right)\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_3}$	$=$	$\left(x_1+\frac{3}{4}\right)\mathbf{a_1}-x_1\,\mathbf{a_2}-x_1\,\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_4}$	$=$	$-x_1\,\mathbf{a_1}+\left(x_1+\frac{3}{4}\right)\mathbf{a_2}+\left(x_1+\frac{3}{4}\right)\mathbf{a_3}$	$=$	$a\left(x_1+\frac{3}{4}\right)\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc I
$\mathbf{B_5}$	$=$	$-\left(x_2-\frac{1}{4}\right)\mathbf{a_1}+x_2\,\mathbf{a_2}+x_2\,\mathbf{a_3}$	$=$	$ax_2\,\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_6}$	$=$	$x_2\,\mathbf{a_1}-\left(x_2-\frac{1}{4}\right)\mathbf{a_2}-\left(x_2-\frac{1}{4}\right)\mathbf{a_3}$	$=$	$-a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{x}}+\frac{1}{8}b\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_7}$	$=$	$\left(x_2+\frac{3}{4}\right)\mathbf{a_1}-x_2\,\mathbf{a_2}-x_2\,\mathbf{a_3}$	$=$	$-ax_2\,\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_8}$	$=$	$-x_2\,\mathbf{a_1}+\left(x_2+\frac{3}{4}\right)\mathbf{a_2}+\left(x_2+\frac{3}{4}\right)\mathbf{a_3}$	$=$	$a\left(x_2+\frac{3}{4}\right)\hat{\mathbf{x}}+\frac{3}{8}b\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Sc II
$\mathbf{B_9}$	$=$	$y_3\,\mathbf{a_1}-\left(y_3-\frac{1}{4}\right)\mathbf{a_2}+y_3\,\mathbf{a_3}$	$=$	$\frac{1}{8}a\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{10}}$	$=$	$-\left(y_3-\frac{1}{4}\right)\mathbf{a_1}+y_3\,\mathbf{a_2}-\left(y_3-\frac{1}{4}\right)\mathbf{a_3}$	$=$	$\frac{1}{8}a\,\hat{\mathbf{x}}-b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{11}}$	$=$	$-y_3\,\mathbf{a_1}+\left(y_3+\frac{3}{4}\right)\mathbf{a_2}-y_3\,\mathbf{a_3}$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{12}}$	$=$	$\left(y_3+\frac{3}{4}\right)\mathbf{a_1}-y_3\,\mathbf{a_2}+\left(y_3+\frac{3}{4}\right)\mathbf{a_3}$	$=$	$\frac{3}{8}a\,\hat{\mathbf{x}}+b\left(y_3+\frac{3}{4}\right)\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	S I
$\mathbf{B_{13}}$	$=$	$(-x_4+y_4+z_4)\,\mathbf{a_1}+(x_4-y_4+z_4)\,\mathbf{a_2}+(x_4+y_4-z_4)\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{14}}$	$=$	$(x_4-y_4+z_4)\,\mathbf{a_1}+(-x_4+y_4+z_4)\,\mathbf{a_2}-\left(x_4+y_4+z_4-\frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_4-\frac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_4-\frac{1}{4}\right)\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{15}}$	$=$	$(x_4+y_4-z_4)\,\mathbf{a_1}-\left(x_4+y_4+z_4-\frac{1}{2}\right)\mathbf{a_2}+(-x_4+y_4+z_4)\,\mathbf{a_3}$	$=$	$-a\left(x_4-\frac{1}{4}\right)\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{16}}$	$=$	$-\left(x_4+y_4+z_4-\frac{1}{2}\right)\mathbf{a_1}+(x_4+y_4-z_4)\,\mathbf{a_2}+(x_4-y_4+z_4)\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}}-b\left(y_4-\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{17}}$	$=$	$(x_4-y_4-z_4)\,\mathbf{a_1}-(x_4-y_4+z_4)\,\mathbf{a_2}-(x_4+y_4-z_4)\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{18}}$	$=$	$-(x_4-y_4+z_4)\,\mathbf{a_1}+(x_4-y_4-z_4)\,\mathbf{a_2}+\left(x_4+y_4+z_4+\frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_4+\frac{1}{4}\right)\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{19}}$	$=$	$-(x_4+y_4-z_4)\,\mathbf{a_1}+\left(x_4+y_4+z_4+\frac{1}{2}\right)\mathbf{a_2}+(x_4-y_4-z_4)\,\mathbf{a_3}$	$=$	$a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S II
$\mathbf{B_{20}}$	$=$	$\left(x_4+y_4+z_4+\frac{1}{2}\right)\mathbf{a_1}-(x_4+y_4-z_4)\,\mathbf{a_2}-(x_4-y_4+z_4)\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}}+b\left(y_4+\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	S II

References

[1] J. P. Dismukes and J. G. White, *The Preparation, Properties, and Crystal Structures of Some Scandium Sulfides in the Range Sc_2S_3-ScS*, Inorg. Chem. **3**, 1220–1228 (1964), doi:10.1021/ic50019a004.